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A QUOTIENT-DIFFERENCE ALGORITHM FOR THE DETERMINATION OF EIGENVALUES OF PERIODIC TRIDIAGONAL MATRICES

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Abstract—A generalised sparse factorisation of periodic tridiagonal matrices was introduced in Evans and Okolie[1]. By applying a similar factorisation strategy in a similarity transformation we obtain a sparse form extension of the Rutishauser's[2] L.R. and Q.D. schemes to determine the eigenvalues of a wide class of symmetric periodic tridiagonal matrices under certain diagonal dominance conditions. The method proposed is recommended for use in practical applications such as in the solution of the self-adjoint periodic characteristic Sturm Liouville problem.

1. INTRODUCTION

Many practical applications, such as the model analysis of floquet waves in composite materials (Yang *et al.*[3]), often involves the solution of the Sturm Liouville eigenvalue problem in the form,

$$\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y+\lambda r(x)y=0, \tag{1.1}$$

$$q(x),\ r(x)>0,\ p(x)\neq 0$$

where we seek the numerical values of λ in a given range R: $a\leqslant x\leqslant b$, subject to the boundary conditions,

$$\left.\begin{aligned} y(a)&=y(b)\\ p(a)\frac{dy(a)}{dx}&=p(b)\frac{dy(b)}{dx}. \end{aligned}\right\} \tag{1.2}$$

If we apply the standard second order finite difference approximation to (1.1) and assume that $p(x)$, $q(x)$ and $r(x)$ are periodic functions with period n, i.e.

$$p_{n+i}=p_i,\quad q_{n+i}=q_i,\quad r_{n+i}=r_i, \tag{1.3}$$

then we obtain the matrix eigenvalue problem (Evans[4]), of the form,

$$A\mathbf{u}=\lambda\mathbf{u} \tag{1.4}$$

where A is an $(n\times n)$ real, symmetric periodic tridiagonal matrix of the form,

$$A=\begin{bmatrix} b_1 & a_2 & & & a_1\\ a_2 & b_2 & a_3 & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & a_n\\ a_1 & & & a_n & b_n \end{bmatrix}. \tag{1.5}$$

In this paper we shall apply a cyclic factorisation of the coefficient matrix to a sparse form extension of a Rutishauser's LR-type similarity transformation, from which the eigenvalues of the matrix A are obtained.

2. DERIVATION OF THE ALGORITHMIC SOLUTION

The fundamental notion of the LR and its variant, the quotient-difference (QD) scheme for the determination of the eigenvalues of a given square matrix is well known[5, 6]. Here, we introduce a sparse form extension of this method to determine the eigenvalues of a periodic symmetric tridiagonal matrix of the form in (1.5) which is assumed to satisfy certain diagonal dominance conditions specified in Section 4. The strategy involves the application of a sparse cyclic factorisation of the coefficient matrix instead of the usual LU decomposition.

Initially, it is convenient to reduce the matrix A to an unsymmetric form by a simple similarity transformation to obtain,

$$A^{(1)} = DAD^{-1} = \begin{bmatrix} b_1^{(1)} & 1 & & & a_1^{(1)} \\ a_2^{(1)} & b_2^{(1)} & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & 1 \\ 1 & & & a_n^{(1)} & b_n^{(1)} \end{bmatrix}_{(n\times n)} \tag{2.1}$$

where,

$$a_i^{(1)} = a_i^2, \quad b_i^{(i)} = b_i, \quad i = 1, 2, \ldots, n; \tag{2.2}$$

and D is a suitable non-singular diagonal matrix. Then, on applying the P–Q cyclic factorisation (Evans and Okolie[1]), we have

$$A^{(1)} = P^{(1)}Q^{(1)} \tag{2.3}$$

where,

$$P^{(1)} = \begin{bmatrix} 1 & & & l_1^{(1)} \\ l_2^{(1)} & 1 & & 0 \\ & \ddots & \ddots & \\ 0 & & \ddots & \\ & & l_n^{(1)} & 1 \end{bmatrix}_{(n\times n)}, \qquad Q^{(1)} = \begin{bmatrix} u_1^{(1)} & 1 & & \\ & u_2^{(1)} & \ddots & 0 \\ & & \ddots & \ddots \\ & 0 & & \ddots & 1 \\ 1 & & & & u_n^{(1)} \end{bmatrix}_{(n\times n)} \tag{2.4}$$

and

$$\left.\begin{aligned} l_i^{(1)} &= a_i^{(1)}/u_{i-1}^{(1)} \\ u_i^{(1)} &= b_i^{(1)} - l_i^{(1)} \end{aligned}\right\} ,i = 1, 2, \ldots, n \text{ and } u_0^{(1)} \equiv u_n^{(1)}. \tag{2.5}$$

The merit of the cyclic factorisation in (2.3) is that both the sparsity and the banded structure of the coefficient matrix A are preserved. However, the elements $l_i^{(1)}$, $u_i^{(1)}$ in (2.5) cannot be determined uniquely unless one element, typically $l_1^{(1)}$ is obtained first in an efficient manner. A continued fraction approach will be adopted for this purpose and given in Section 3.

Next, by following the LR-type transformation, we re-multiply $P^{(1)}$ and $Q^{(1)}$ in the reverse order to give,

$$A^{(2)} = Q^{(1)}P^{(1)} \tag{2.6}$$

or

$$\begin{bmatrix} b_1^{(2)} & 1 & & & a_1^{(2)} \\ a_2^{(2)} & b_2^{(2)} & 1 & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & 1 \\ 1 & & & a_n^{(2)} & b_n^{(2)} \end{bmatrix} = \begin{bmatrix} u_1^{(1)}+l_2^{(1)} & 1 & & & u_1^{(1)}l_1^{(1)} \\ u_2^{(1)}l_2^{(1)} & u_2^{(1)}+l_3^{(1)} & 1 & & 0 \\ & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & 1 \\ 1 & & & u_n^{(1)}l_n^{(1)} & u_n^{(1)}+l_1^{(1)} \end{bmatrix} \tag{2.7}$$

from which we derive,

$$\left.\begin{aligned} b_i^{(2)} &= u_i^{(1)} + l_{i+1}^{(1)} \\ a_i^{(2)} &= u_i^{(1)} l_i^{(1)} \end{aligned}\right\} \quad i = 1, 2, \ldots, n \text{ and } l_{n+1}^{(1)} \equiv l_1^{(1)}. \tag{2.8}$$

A further cyclic factorisation of $A^{(2)}$ gives,

$$A^{(2)} = P^{(2)} Q^{(2)} \tag{2.9}$$

from which we obtain a set of equations analogous to (2.5) and given by,

$$\left.\begin{aligned} l_i^{(2)} &= a_i^{(2)} / u_{i-1}^{(2)} \\ u_i^{(2)} &= b_i^{(2)} - l_i^{(2)} \end{aligned}\right\} \quad i = 1, 2, \ldots, n,\ u_0^{(2)} \equiv u_n^{(2)}. \tag{2.10}$$

A substitution of (2.8) into (2.10) leads to the relations

$$l_i^{(2)} = u_i^{(1)} l_i^{(1)} / u_{i-1}^{(2)}$$

and

$$\left. u_i^{(2)} = u_i^{(1)} + l_{i+1}^{(1)} - l_i^{(2)} \right\} \quad i = 1, 2, \ldots, n \tag{2.11}$$

with

$$l_{n+1}^{(2)} = l_1^{(2)}, \quad u_0^{(2)} \equiv u_n^{(2)}.$$

Generally, at the sth stage of the LR-type transformation, a remultiplication followed by a decomposition, i.e.

$$A^{(s)} = Q^{(s-1)} P^{(s-1)}$$

and

$$A^{(s)} = P^{(s)} Q^{(s)} \tag{2.12}$$

yields elements of $P^{(s)}$ and $Q^{(s)}$ such that,

$$l_i^{(s)} = u_i^{(s-1)} l_i^{(s-1)} / u_{i-1}^{(s)}$$

and

$$\left. u_i^{(s)} = u_i^{(s-1)} + l_{i+1}^{(s-1)} - l_i^{(s)} \right\} \quad i = 1, 2, \ldots, n; \quad s = 2, 3, \ldots \tag{2.13}$$

with

$$l_{n+1}^{(s)} = l_1^{(s)}, \; u_0^{(s)} \equiv u_n^{(s)}.$$

The first and second equations in (2.13) are analogous to the well-known rhombus rules [6] and may be denoted as the periodic quotient and difference rules, respectively.

Table 1. The periodic quotient difference table

$\ell_1^{(1)}$					
$u_1^{(1)}$					
$\ell_1^{(2)}$	$\ell_2^{(1)}$				
$u_1^{(2)}$	$u_2^{(1)}$				
$\ell_1^{(3)}$	$\ell_2^{(2)}$	$\ell_3^{(1)}$			
$u_1^{(3)}$	$u_2^{(2)}$	$u_3^{(1)}$			
$\ell_1^{(4)}$	$\ell_2^{(3)}$	$\ell_3^{(2)}$	$\ell_4^{(1)}$		
$u_1^{(4)}$	$u_2^{(3)}$	$u_3^{(2)}$	$u_4^{(1)}$		
$\ell_1^{(5)}$	$\ell_2^{(4)}$	$\ell_3^{(3)}$	$\ell_4^{(2)}$	$\ell_5^{(1)}$	
$u_1^{(5)}$	$u_2^{(4)}$	$u_3^{(3)}$	$u_4^{(2)}$	$u_5^{(1)}$	
$\ell_1^{(6)}$	$\ell_2^{(5)}$	$\ell_3^{(4)}$	$\ell_4^{(3)}$	$\ell_5^{(2)}$	$\ddots$
$u_1^{(6)}$	$u_2^{(5)}$	$u_3^{(4)}$	$u_4^{(3)}$	$u_5^{(2)}$	$\ddots$
$\ell_1^{(7)}$	$\ell_2^{(6)}$	$\ell_3^{(5)}$	$\ell_4^{(4)}$	$\ell_5^{(3)}$	$\ddots$
$u_1^{(7)}$	$u_2^{(6)}$	$u_3^{(5)}$	$u_4^{(4)}$	$u_5^{(3)}$	
	$\ell_2^{(7)}$	$\ell_3^{(6)}$	$\ell_4^{(5)}$	$\ell_5^{(4)}$	$\ddots$
	$u_2^{(7)}$	$u_3^{(6)}$	$u_4^{(5)}$	$u_5^{(4)}$	
	$\ddots$	$\ddots$	$\ddots$	$\ddots$	

A combination of equations (2.5) and (2.13) constitute the periodic quotient-difference (PQD) scheme which may be arranged in the form given in Table 1.

The convergence of the LR (and QD) schemes for the determination of eigenvalues of positive definite matrices is well known[5, 6]. The PQD scheme presented here is a variant of the QD algorithm and hence the convergence proof of the former is adequately covered in Wilkinson[5]. This implies that the $u_i^{(s)}$ terms of the PQD chart converge to the eigenvalues of $A^{(1)}$ and also that the $l_i^{(s)}$ terms converge to zero as s tends to infinity. It may also be mentioned that the well-known acceleration techniques including the shift of origin and deflation, which are usually applied in the LR method can equally be applied to the proposed PQD scheme. However, it is necessary to evaluate a periodic continued fraction at each step of the LR-type transformation of the proposed method, the coefficient matrix is also required to satisfy additional conditions in order to guarantee the convergence of the continued fractions and hence that of the PQD scheme.

3. DETERMINATION OF $l_1^{(s)}$ BY A CONTINUED FRACTION EXPANSION

At each step of the PQD scheme, an element, preferably $l_1^{(s)}$ $(s = 1, 2, \ldots)$ must be determined first in an efficient manner before the other elements $l_i^{(s)}$, $u_i^{(s)}$ in (2.5) and (2.13) can be uniquely obtained.

For $s = 1$, the $l_1^{(s)}$ is derived as an infinite periodic continued fraction by a cyclic application of equation (2.5) to give, using the standard continued fraction notation

$$l_1^{(1)} = \underbrace{\frac{a_1^{(1)}}{b_n^{(1)}-}\frac{a_n^{(1)}}{b_{n-1}^{(1)}-}\frac{a_{n-1}^{(1)}}{b_{n-2}^{(1)}-}\cdots\frac{a_2^{(1)}}{b_1^{(1)}-}}_{\text{1st cycle}}\underbrace{\frac{a_1^{(1)}}{b_n^{(1)}-}\frac{a_n^{(1)}}{b_{n-1}^{(1)}-}\frac{a_{n-1}^{(1)}}{b_{n-2}^{(1)}-}\cdots\frac{a_2^{(1)}}{b_1^{(1)}-}}_{\text{2nd cycle}}\underbrace{\frac{a_1^{(1)}}{b_n^{(1)}-}\cdots}_{\text{etc.}} \tag{3.1}$$

Equation (3.1) can be written in the general form,

$$l_1^{(1)} = \frac{\alpha_1}{\beta_1-}\frac{\alpha_2}{\beta_2-}\frac{\alpha_3}{\beta_3-}\cdots\frac{\alpha_n}{\beta_n-}\frac{\alpha_1}{\beta_1-}\frac{\alpha_2}{\beta_2-}\cdots\frac{\alpha_n}{\beta_n-}\frac{\alpha_1}{\beta_1-}\cdots \tag{3.2}$$

where

$$\left.\begin{aligned}\alpha_i &= a^{(1)}_{(n-i+2)}\\ \beta_i &= b^{(1)}_{(n-i+1)}\end{aligned}\right\} i = 1,2,\dots,n \text{ and } (k) \equiv k(\text{modulo } n). \tag{3.3}$$

The infinite periodic continued fraction (3.2) is said to be generated by the *linear fractional transformation*,

$$\tau^{(n)}(\omega) = \frac{\alpha_1}{\beta_1}\text{-}\frac{\alpha_2}{\beta_2}\text{-}\frac{\alpha_3}{\beta_3}\text{-}\cdots\frac{\alpha_n}{\beta_n - \omega} \tag{3.4}$$

where ω is the *fixed point* of the transformation at infinity[7].

Similarly, for $s = 2,3,\dots, l_1^{(s)}$ is derived as an infinite continued fraction by a cyclic application of (2.11) to give,

$$l_1^{(s)} = \underbrace{\frac{u_1^{(s-1)}l_1^{(s-1)}}{u_n^{(s-1)}+l_1^{(s-1)}}\text{-}\frac{u_n^{(s-1)}l_n^{(s-1)}}{u_{n-1}^{(s-1)}+l_n^{(s-1)}}\text{-}\frac{u_{n-1}^{(s-1)}l_{n-1}^{(s-1)}}{u_{n-2}^{(s-1)}+l_{n-1}^{(s-1)}}\text{-}\cdots\frac{u_2^{(s-1)}l_2^{(s-1)}}{u_1^{(s-1)}+l_2^{(s-1)}}\text{-}}_{\text{1st cycle}}$$

$$\underbrace{\frac{u_1^{(s-1)}l_1^{(s-1)}}{u_n^{(s-1)}+l_1^{(s-1)}}\text{-}\frac{u_n^{(s-1)}l_n^{(s-1)}}{u_{n-1}^{(s-1)}+l_n^{(s-1)}}\text{-}\frac{u_{n-1}^{(s-1)}l_{n-1}^{(s-1)}}{u_{n-2}^{(s-1)}+l_{n-1}^{(s-1)}}\text{-}\cdots\frac{u_2^{(s-1)}l_2^{(s-1)}}{u_1^{(s-1)}+l_2^{(s-1)}}\text{-}}_{\text{2nd cycle}}\frac{u_1^{(s-1)}l_1^{(s-1)}}{u_n^{(s-1)}+l_1^{(s-1)}}\text{-}\cdots \tag{3.5}$$

which we can also rewrite in the standard form (3.2) where in this case,

$$\left.\begin{aligned}\alpha_i &= l_{(n-i+2)}u_{(n-i+2)}\\ \beta_i &= l_{(n-i+2)} + u_{(n-i+1)}\end{aligned}\right\} i = 1,2,\dots,n; \quad (k) \equiv k(\text{modulo } n). \tag{3.6}$$

The periodic continued fraction in (3.1) and (3.5) is guaranteed to converge provided the coefficient matrix satisfies the conditions specified later in (4.8).

Furthermore, the value of the infinite continued fraction (3.2) is given by Wall[7]

$$l_1^{(s)} = \max(\omega_1, \omega_2)$$

where ω_1, ω_2 are the fixed points of the linear fractional transformation (3.4) and their values are obtained from the solution of the quadratic equation

$$\omega = \frac{E_{k-1}\omega + E_k}{F_{k-1}\omega + F_k} \tag{3.8}$$

where

$$\left.\begin{aligned}&E_0 = 0, \quad F_0 = 1,\\ &E_1 = \alpha_1, \quad F_1 = \beta_1,\\ &\left.\begin{aligned}E_r &= \beta_r E_{r-1} - \alpha_r E_{r-2}\\ F_r &= \beta_r F_{r-1} - \alpha_r F_{r-2}\end{aligned}\right\} r = 2,3,\dots,k \leqslant n.\end{aligned}\right\} \tag{3.9}$$

and

The quotient E_r/F_r is the r^{th} approximant of the continued fraction in (3.2); and the sequence of approximants $\{E_r/F_r\}$ is said to converge after the kth approximant if

$$\left|\frac{E_k}{F_k} - \frac{E_{k-1}}{F_{k-1}}\right| < \epsilon \tag{3.10}$$

for a sufficiently small truncation error tolerance $\epsilon(\simeq 10^{-12})$.

It is observed that for matrices which satisfy the diagonal dominance condition (4.8) the series of approximants of the continued fraction of the form (3.1) or (3.5) form a rapidly convergent sequence; and as a general rule each additional approximant yields one further correct decimal place. Hence, the convergence criterion in (3.9) is usually satisfied after the order of t levels of recursion, where t is the maximum number of decimal place accuracy of the computer. It is therefore only necessary to evaluate the recurrence relation to a level $k = t \leq n$ where 10^{-t} is an acceptable truncation error tolerance. This indicates that the computing effort required to determine $l_1^{(s)}$ by the continued fraction approach is relatively inexpensive, particularly for cases where n, the order of the coefficient matrix, is large.

4. CONVERGENCE OF THE INFINITE CONTINUED FRACTION

We consider a periodic tridiagonal matrix $A^{(s)}$ of the form,

$$A^{(s)} = \begin{bmatrix} b_1^{(s)} & c_1^{(s)} & & & a_1^{(s)} \\ a_2^{(s)} & b_2^{(s)} & c_2^{(s)} & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & c_{n-1}^{(s)} \\ c_n^{(s)} & & & a_n^{(s)} & b_n^{(s)} \end{bmatrix} \tag{4.1}$$

and associated with the cyclic factorisation of this matrix we define an infinite continued fraction of the form,

$$\Gamma_A = \frac{\alpha}{\beta_1 -}\frac{\alpha_2}{\beta_2 -}\frac{\alpha_3}{\beta_3 -}\cdots\frac{\alpha_n}{\beta_n -}\frac{\alpha_1}{\beta_1 -}\frac{\alpha_2}{\beta_2 -}\frac{\alpha_3}{\beta_3 -}\cdots\frac{\alpha_n}{\beta_n -}\cdots \tag{4.2}$$

where in general,

$$\left.\begin{aligned} \alpha_i &= a^{(s)}_{(n-i+2)}c^{(s)}_{(n-i+1)} \\ \beta_i &= b^{(s)}_{(n-i+1)} \end{aligned}\right\} \quad i = 1, 2, \ldots, n \text{ and } (j) \equiv j(\text{modulo } n). \tag{4.3}$$

It is now necessary to establish the form of the matrix $A^{(s)}$ in (4.1) for which the associated infinite continued fraction (4.2) is always guaranteed to converge. The following well known theorems are essential for this purpose.

Theorem 1. A continued fraction is unchanged in value if some partial numerator and partial demonimator, along with the immediate succeeding partial numerator, are multiplied by the same non-zero constant.

The proof of the above theorem is given in Wall[7] and is termed an equivalence transformation.

Theorem 2. A sufficient condition for the convergence of a continued fraction of the form,

$$\Gamma_B = \frac{\theta}{1 -}\frac{\theta_2}{1 -}\frac{\theta_3}{1 -}\cdots\frac{\theta_n}{1 -}\frac{\theta_1}{1 -}\frac{\theta_2}{1 -}\frac{\theta_3}{1 -}\cdots\frac{\theta_n}{1 -}\cdots \tag{4.4}$$

is that $0 \leq \theta_i \leq \frac{1}{4}$. (4.5)

The proof of Theorem 2 is given in Blanch, [8].

Now, by a successive application of Theorem 1, the continued fraction in (4.2) can be transformed into the form in (4.4) where,

$$\left.\begin{aligned} &\theta_1 = \frac{\alpha_1}{\beta_1} \\ \text{and} \\ &\theta_i = \alpha_i/(\beta_{i-1}\beta_i), \quad \beta_{i-1}, \beta_i \neq 0, \quad i = 2, 3, \ldots, n. \end{aligned}\right\} \tag{4.6}$$

On applying Theorem 2 and substituting for θ_i from (4.6), it follows immediately that the continued fraction in (4.2) converges if

$$\left.\begin{aligned} &0 \leq \alpha_1/\beta_1 \leq 0 \\ \text{and} \\ &0 \leq \alpha_i/(\beta_{i-1}\beta_i) \leq \frac{1}{4}, \quad i = 2, 3, \ldots, n. \end{aligned}\right\} \tag{4.7}$$

Further, on substituting for α_i, β_i from (4.3), we obtain the final conditions, involving elements of $A^{(s)}$ as,

$$\left.\begin{aligned} &0 \leq \frac{a_1^{(s)} c_n^{(s)}}{b_n^{(s)}} \leq \frac{1}{4} \\ &0 \leq \frac{a_{(n-i+2)}^{(s)}}{b_{(n-i+2)}^{(s)}} \frac{c_{(n-i+1)}^{(s)}}{b_{(n-i+1)}^{(s)}} \leq \frac{1}{4}, \quad i = 2, 3, \ldots, n. \end{aligned}\right\} \tag{4.8}$$

Thus, we have shown that for any matrix $A^{(s)}$ of the form in (4.1), a sufficient condition for the convergence of the associated infinite continued fraction obtained as a result of a cyclic factorisation of $A^{(s)}$ is given by conditions (4.8).

The relation in (4.8) is a ratio. It means that if a given matrix $A^{(1)}$ (say) satisfies condition (4.8), then any other matrix $A^{(s)}$, $s = 2, 3, \ldots,$ which is similar to $A^{(1)}$ will necessarily satisfy (4.8). Thus, for practical purposes, it is only necessary to verify that any given coefficient matrix A satisfies condition (4.8) before the application of the proposed PQD method.

5. NUMERICAL RESULTS

The PQD algorithm presented in Section 2 was programmed in Fortran using single precision arithmetic and run on the Loughborough University I.C.L. 1904S computer.

We consider as an example the (10×10) symmetric periodic tridiagonal matrix,

$$A = \begin{bmatrix} 4 & 1 & & & & 1 \\ 1 & 6 & 1 & & 0 & \\ & 1 & 8 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & \ddots & 1 \\ 1 & & & & 1 & 22 \end{bmatrix}_{(10 \times 10)} \tag{5.1}$$

which is positive definite and satisfies condition (4.8). The eigenvalues of the matrix A obtained by using the PQD algorithm were compared with those given by the Nottingham Algorithm Group (N.A.G.) library routine F02AFF (which computes the eigenvalues by the QR method).

The results are given in Table 2 and both are in agreement within an accuracy of 7 significant figures.

Table 2. The eigenvalues of a periodic tridiagonal matrix

i	PQD Algorithm λ_i	N.A.G.(FO2AFF) Routine λ_i
1	3.504298196	3.504298100
2	5.943003306	5.943003271
3	7.997003770	7.997003268
4	9.999922587	9.999923084
5	11.999998885	11.999997609
6	14.000001193	14.000002391
7	16.000077639	16.000076916
8	18.002996412	18.002996733
9	20.056996807	20.056996730
10	22.495701134	22.495701899

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